Supplementary materials

Effect of Aggregation and Adsorption Behavior on the Flow Resistance of Surfactant Fluid on Smooth and Rough Surfaces: A Many-Body Dissipative Particle Dynamics Study

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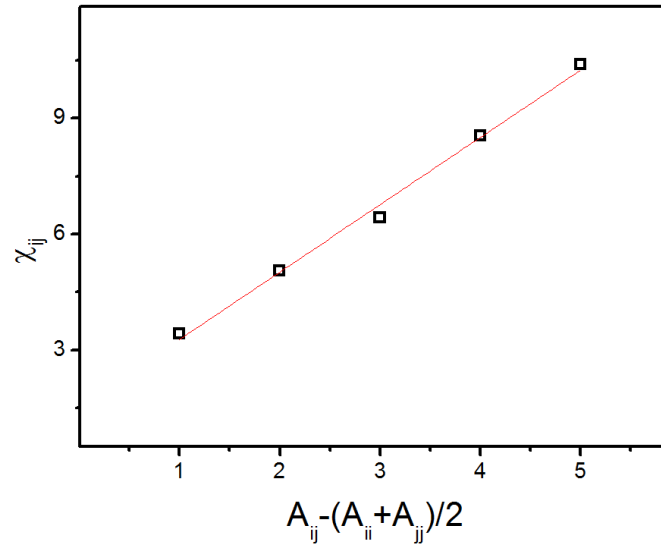
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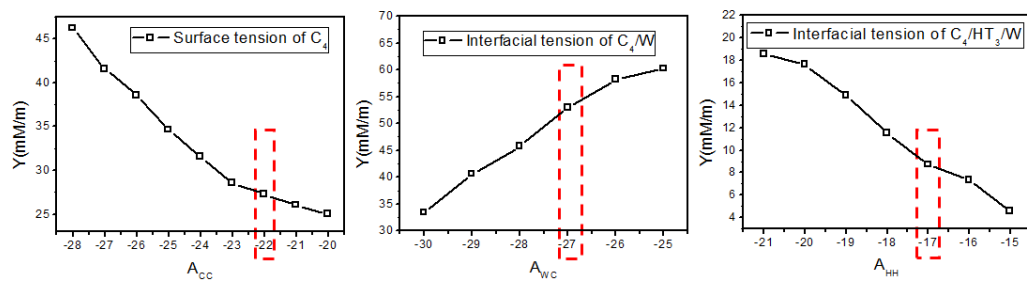
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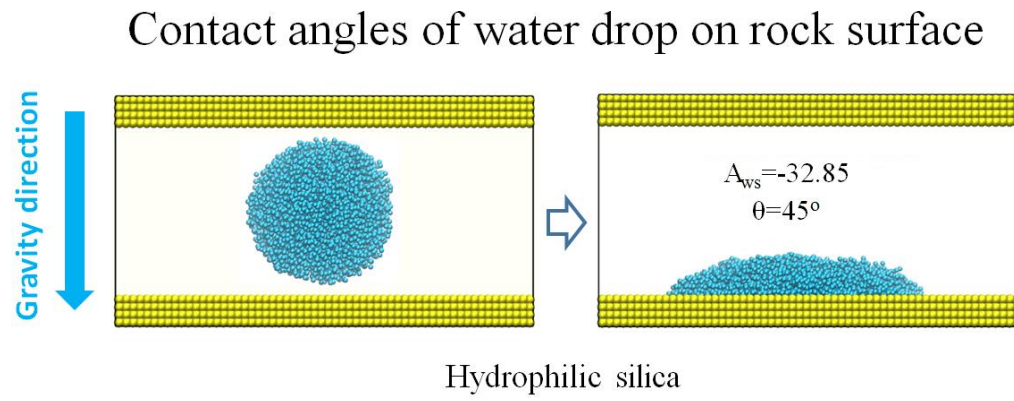
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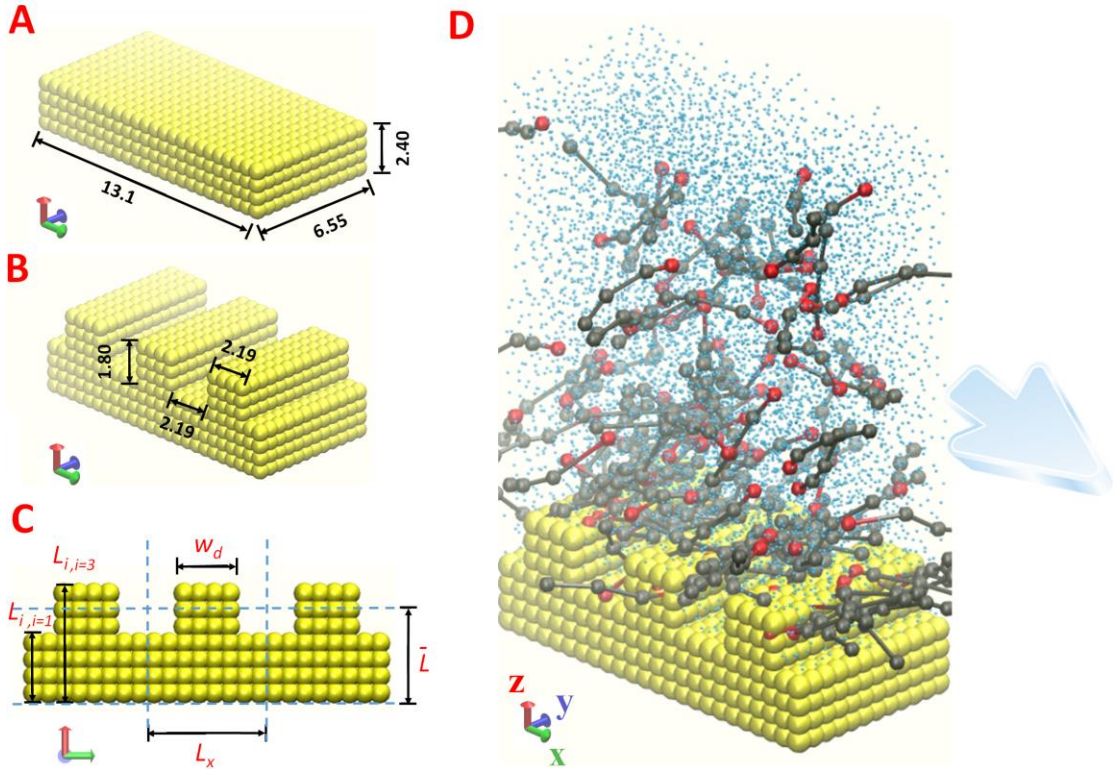E-mail addresses: houjian@upc.edu.cn.

Figure S1. $2\alpha\rho(A_{ij}-(A_{ii}+A_{jj})/2)$ as function of χ_{ij} from a linear function. $2\alpha\rho$ was measured to be 2.138. As a result, $A_{ij}=(A_{ii}+A_{jj})/2+0.469\chi_{ij}$.

Figure S2. Parameterization of A_{CC}, A_{WC} and A_{HH}.

**Figure S3.** Contact angles of the rock surface in MDPD model.

Figure S4. Models of flowing system. (A) Smooth solid surface. (B) Rough solid surface. (C) Definition of surface roughness. The roughness of solid surface is characterized by the normalized surface roughness factors r_x and root-mean-square roughnesses (R), which are defined as $r_x = w_d/L_x$ and $R = [\frac{1}{N}\sum_{i=1}^{N}(Li - \bar{L})^2]^{1/2}$, where L_i is the height of the wall bead i. The values of r_x for smooth and rough surface are 0.00 and 0.50, respectively. The values of R for smooth and rough surface are 0.00 and 0.98 nm, respectively. (D) One snapshot of the flowing system for the surfactant fluid on rough surface. An external driving force of $F_e = 0.02$ was applied on the W beads in the X direction to generalize the continuous flow in the fluid simulation.
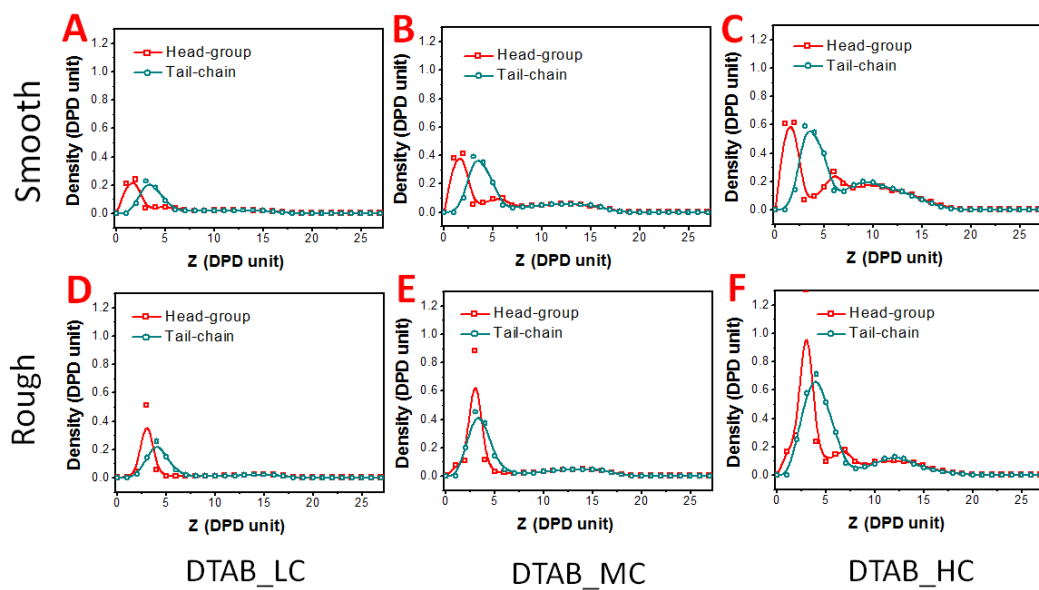
Figure S5. Density profiles of DTAB at 390K on smooth and rough surface in EMDPD simulations. DTAB simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.
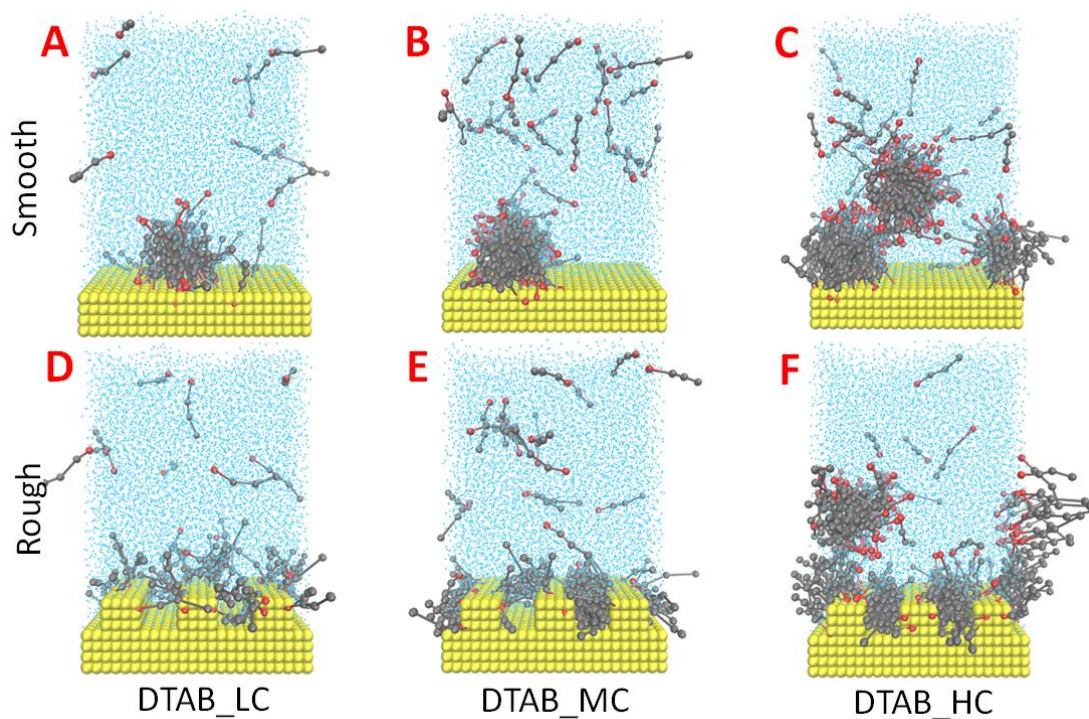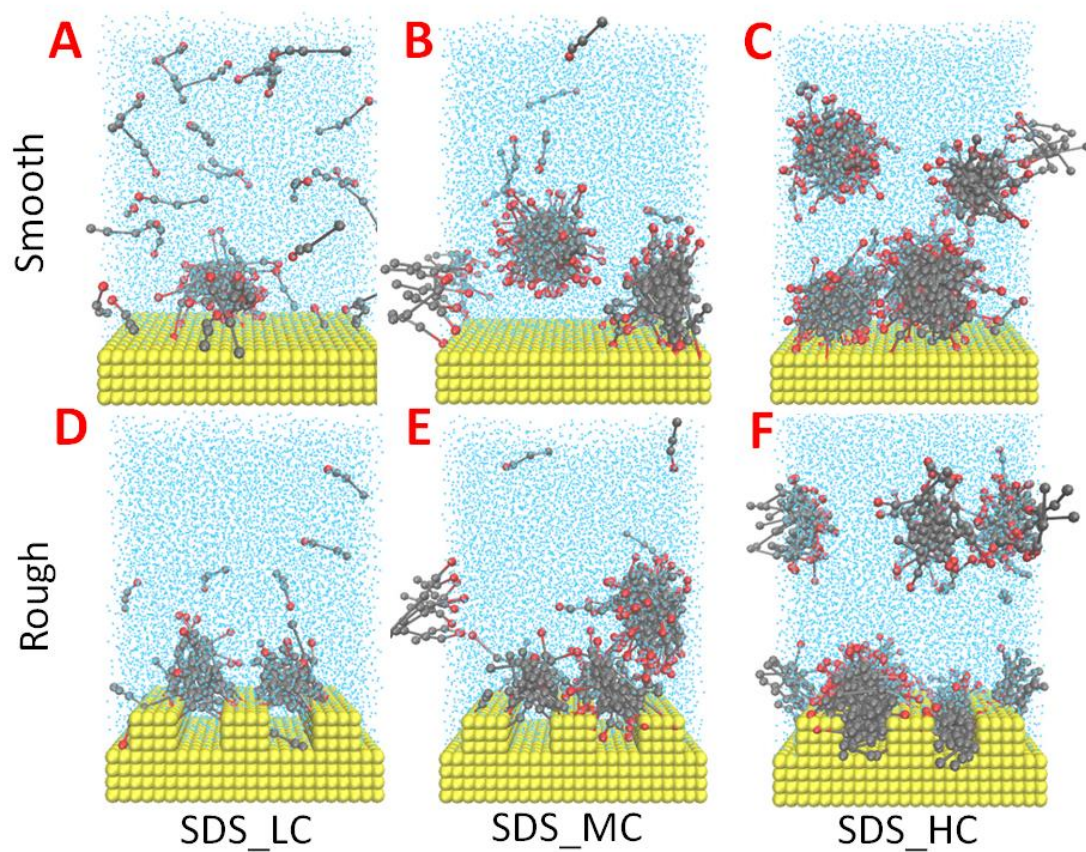
Figure S6. Snapshot of adsorption morphologies of DTAB at 390K on smooth and rough surface in EMDPD simulations. DTAB simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.
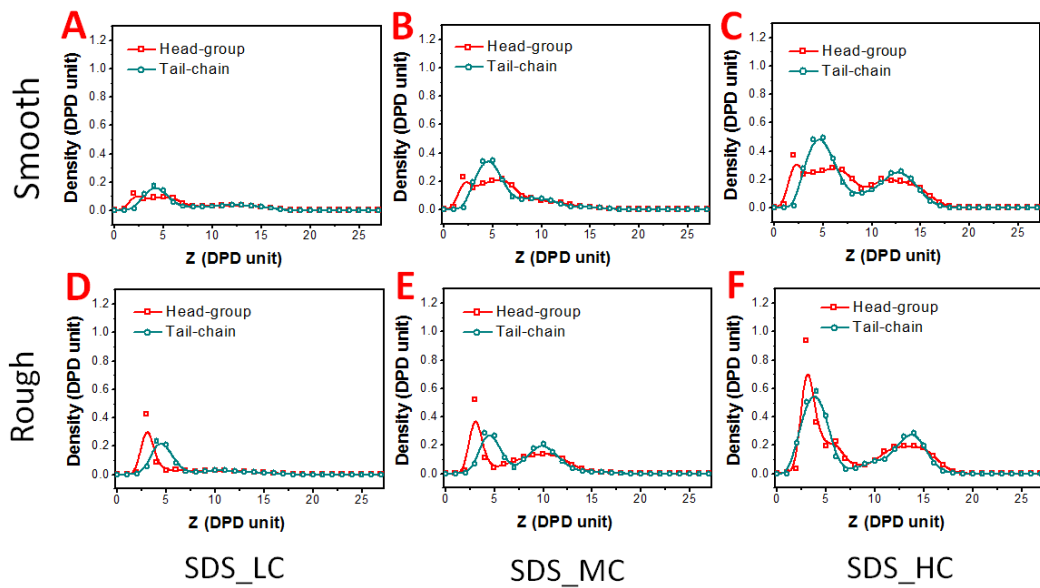
Figure S7. Density profiles of SDS at 300K on smooth and rough surface in EMDPD simulations. SDS simulations at 300K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.

Figure S8. Snapshot of the adsorption morphologies of SDS at 300K on smooth and rough surface in EMDPD simulations. SDS simulations at 300K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.
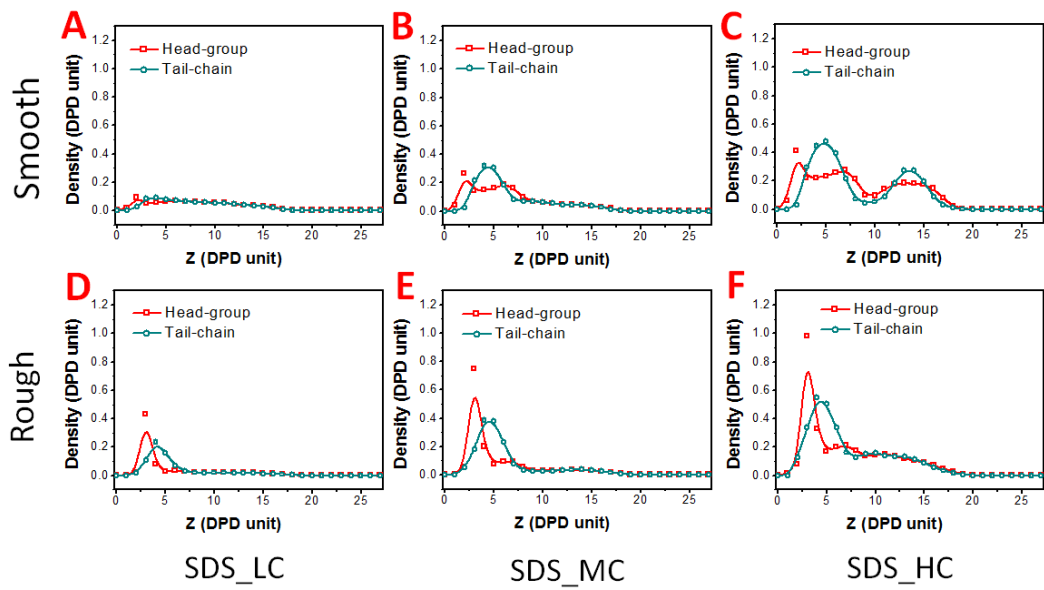
Figure S9. Density profiles of SDS at 390K on smooth and rough surface in EMDPD simulations. SDS simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.

Figure S10. Snapshot of the adsorption morphologies of SDS at 390K on smooth and rough surface in EMDPD simulations. SDS simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.
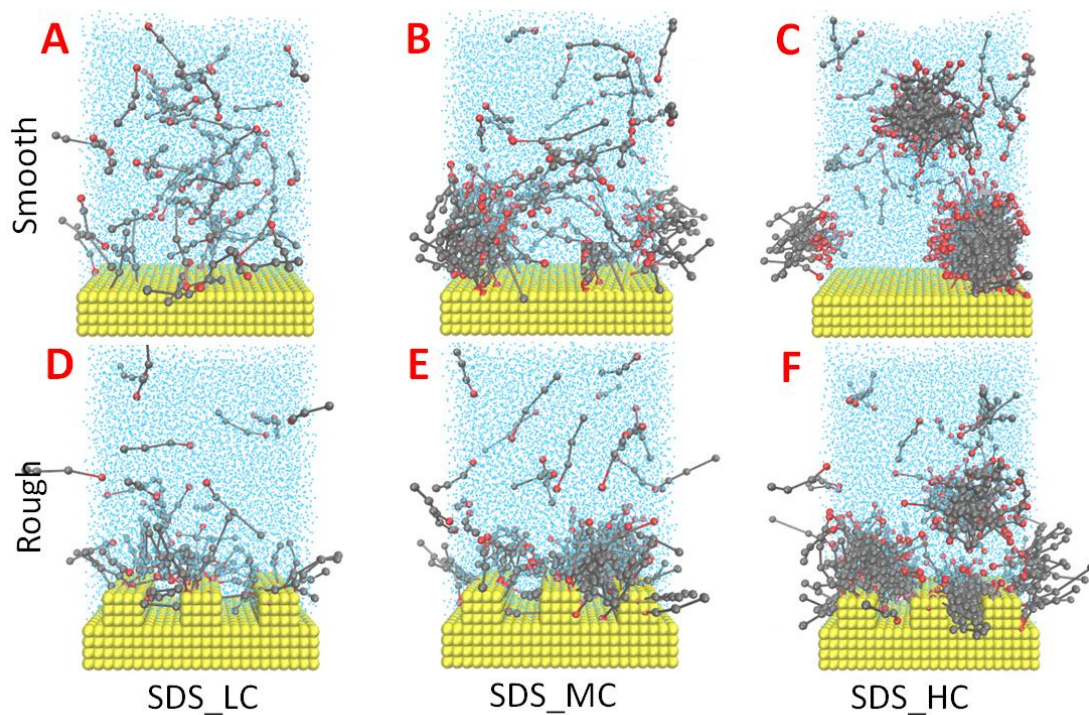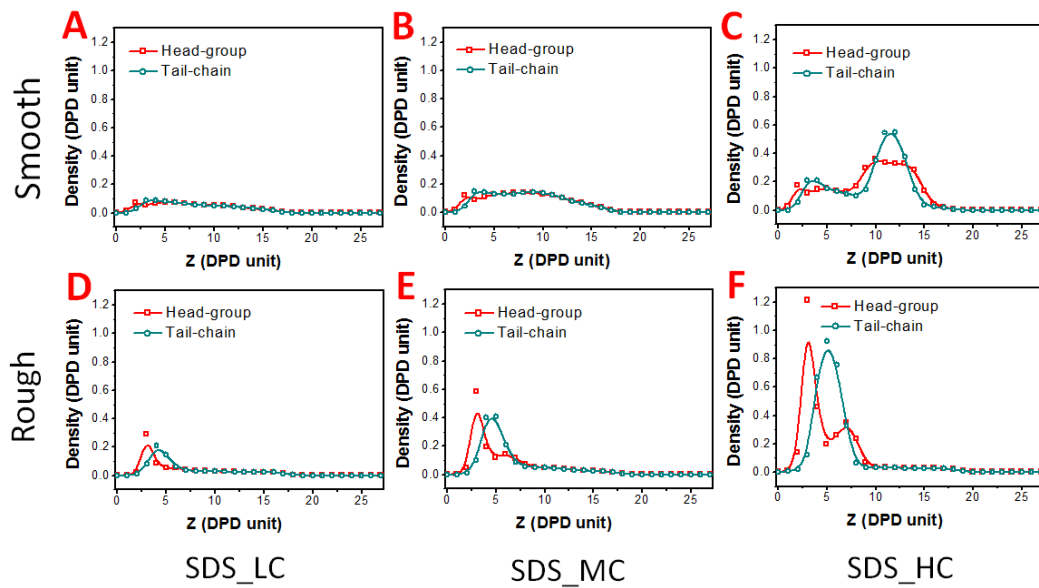
Figure S11. Density profiles of SDS at 390K on smooth and rough surface in NEMDPD simulations. SDS simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.

Figure S12. Snapshot of the adsorption morphologies of SDS at 390K on smooth and rough surface in NEMDPD simulations. SDS simulations at 390K on smooth surface with low (A), medium (B) and high (C) concentrations and rough surface with low (D), medium (E) and high (F) concentrations.
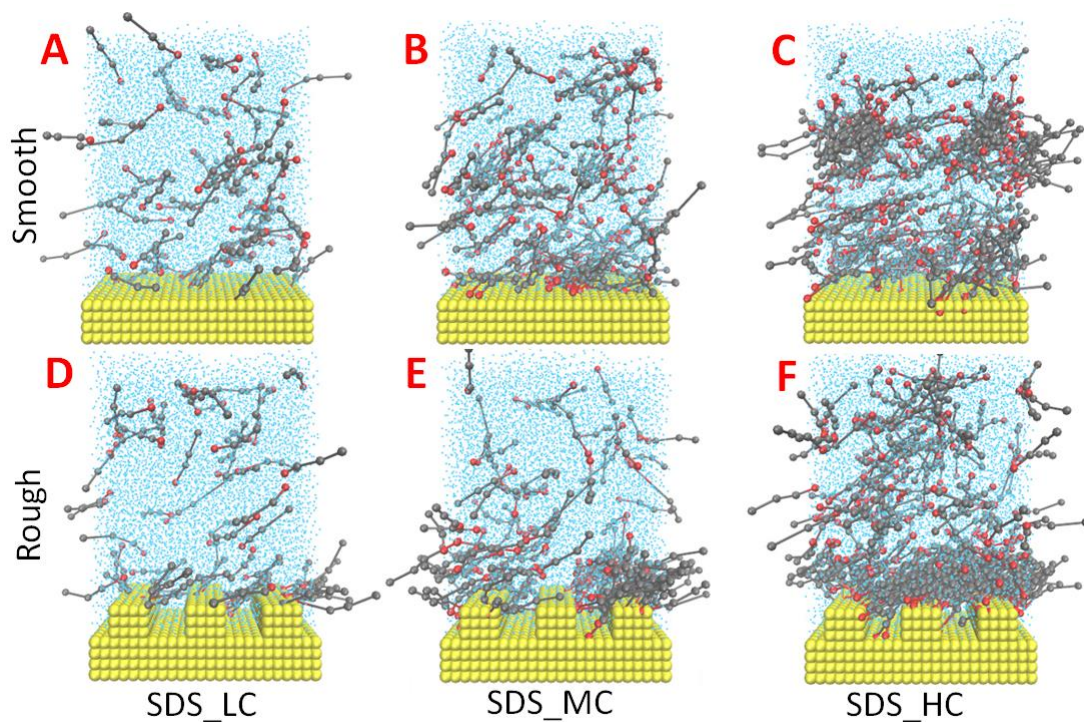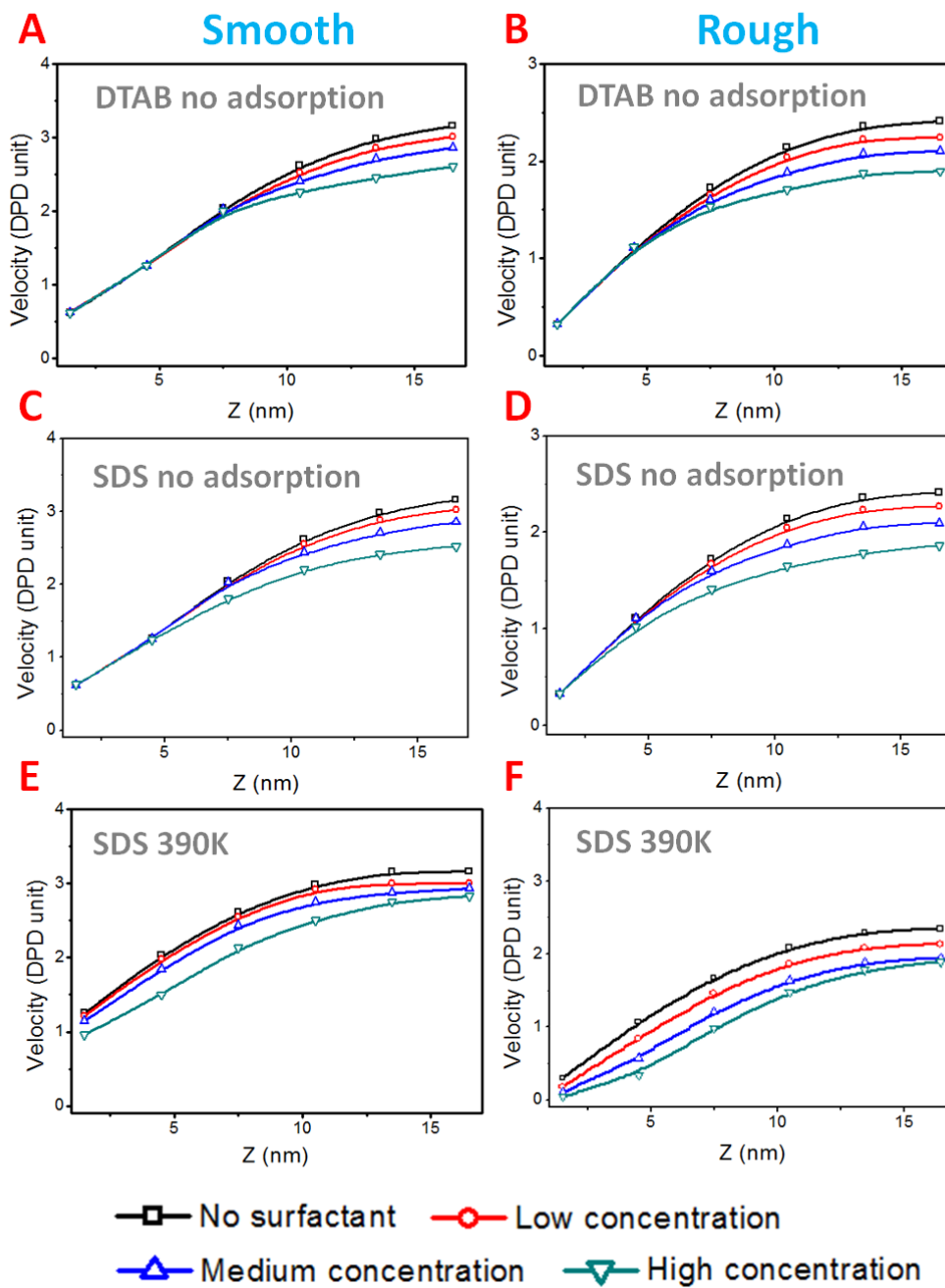
Figure S13. Velocity profile of surfactant fluids on smooth and rough surface in NEMDPD simulations. DTAB on the smooth (A) and rough surface (B) with no adsorption, SDS on the smooth (C) and rough surface (D) with no adsorption and SDS on the smooth (E) and rough surface (F) at 390K.

Table S1. Summary of density distribution of surfactant on the solid surface and fluid bulk phase.

	MD types	Position	Smooth (LC)	Smooth (MC)	Smooth (HC)	Rough (LC)	Rough (MC)	Rough (HC)
DTAB 300K	Static	surface	0.81	1.15	2.19	0.61	1.27	2.69
		bulk phase	0.19	0.85	1.81	0.39	0.73	1.31
	Flow	surface	0.82	1.94	2.81	0.95	1.96	3.94
		bulk phase	0.18	0.06	1.19	0.05	0.04	0.06
DTAB 390K	Static	surface	0.82	1.43	2.50	0.80	1.55	3.02
		bulk phase	0.18	0.57	1.50	0.20	0.45	0.98
	Flow	surface	0.69	1.28	2.42	0.74	1.49	2.43
		bulk phase	0.31	0.72	1.58	0.26	0.51	1.57
SDS 300K	Static	surface	0.66	1.47	2.12	0.77	1.26	2.35
		bulk phase	0.34	0.53	1.88	0.23	0.74	1.65
	Flow	surface	0.53	1.11	1.64	0.79	1.78	2.64
		bulk phase	0.47	0.89	2.36	0.21	0.22	1.36
SDS 390K	Static	surface	0.50	1.38	2.11	0.78	1.40	2.49
		bulk phase	0.50	0.62	1.89	0.22	0.60	1.51
	Flow	surface	0.49	0.91	1.11	0.68	1.35	2.46
		bulk phase	0.51	1.09	2.89	0.32	0.65	1.54

The surfactant molecules within Z=7.5 is defined to be in the adsorption layer on rock surface, and the left surfactant is considered to be in the bulk fluid phase. The amount of surfactant is numerically normalized with low concentration in LC models.